



NRL/FR/7140--05-10,108

A Systematic Approach to Higher-Order Parabolic Propagation in a Weakly Range-Dependent Duct

ROBERT F. GRAGG

*Acoustic Systems Branch
Acoustics Division*

September 28, 2005

Approved for public release; distribution is unlimited.

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.					
1. REPORT DATE (DD-MM-YYYY) 28-09-2005		2. REPORT TYPE Formal Report		3. DATES COVERED (From - To)	
4. TITLE AND SUBTITLE A Systematic Approach to Higher-Order Parabolic Propagation in a Weakly Range-Dependent Duct				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Robert F. Gragg				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Naval Research Laboratory 4555 Overlook Ave Washington, DC 20375-5320				8. PERFORMING ORGANIZATION REPORT NUMBER NRL/FR/7140--05-10,108	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Office of Naval Research 800 N. Quincy Street Arlington, VA 22217-5560				10. SPONSOR / MONITOR'S ACRONYM(S)	
				11. SPONSOR / MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT Energy-conserving transformations are exploited to split a monochromatic field in a weakly inhomogeneous waveguide into a pair of components that undergo uncoupled parabolic propagation in opposite directions along the waveguide axis. A systematic series of such transformations is developed to accomplish this splitting at increasing order of approximation while avoiding backscatter. In order to emphasize fundamentals, this technique is applied in what is arguably the simplest nontrivial case: waves of vertical displacement on a horizontal membrane with a smooth density inhomogeneity along one direction that forms a duct in the orthogonal direction. The evolution of these "drumhead" vibrations is governed by a single continuous environmental variable, the density. This work is meant to serve as a link between an earlier treatment of the simpler, purely one-dimensional case (waves on a string) and the analyses of Wurmser and coworkers of considerably more complex cases featuring multiple environmental variables and/or ducts with discontinuities.					
15. SUBJECT TERMS Parabolic propagation, Order-by-order decoupling, Foldy-Wouthuysen transformations					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UL	18. NUMBER OF PAGES 33	19a. NAME OF RESPONSIBLE PERSON Robert F. Gragg
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (include area code) (202) 404-4816

CONTENTS

1. INTRODUCTION	1
2. BACKGROUND	2
2.1 Membrane Dynamics	2
2.2 Splitting the Helmholtz Equation	3
2.3 State-Space Description	4
3. FURTHER TRANSFORMATIONS	7
3.1 General Environment	7
3.2 Longitudinally Invariant Environment	8
4. MATRIX REPRESENTATIONS	9
4.1 Block-Diagonal $[B]$	12
4.2 Block Off-Diagonal $[B]$	13
5. TRANSFORMING THE GENERATOR	14
5.1 Order $m = 0$	14
5.2 Order $m = 1$	15
5.3 Order $m = 2$	15
5.4 Order $m = 3$	16
5.5 Order $m = 4$	17
6. SUMMARY AND DISCUSSION	19
ACKNOWLEDGMENTS	21
REFERENCES	21
APPENDIX — Details of the Transformations	23

A SYSTEMATIC APPROACH TO HIGHER-ORDER PARABOLIC PROPAGATION IN A WEAKLY RANGE-DEPENDENT DUCT

1. INTRODUCTION

This work deals with a continuous wave (cw; i.e., monochromatic) wave field and focuses on its systematic separation in a ducting environment with weak range dependence into components that propagate in opposite directions along the duct via a hierarchy of uncoupled parabolic equations (PEs). Situations of this general type occur for electromagnetics in the atmosphere and acoustics in the ocean, when very accurate modeling is required for fields that propagate over long ranges through ducts whose range dependence is weak enough that no energy is backscattered.

To highlight the essentials with a minimum of complexity, the simplest nontrivial version of this problem is addressed: waves of vertical (z) displacement on a membrane stretched in the horizontal (x, y) plane. Situations are considered in which the membrane's density has (i) a sufficiently strong maximum in the transverse (y) direction to produce ducting in the longitudinal (x) direction, but (ii) only a weak dependence on the longitudinal coordinate. It is shown that a series of explicitly energy-conserving “pseudounitary” transformations can asymptotically decouple the Helmholtz equation order by order into PEs for left- and right-going ($-x$ and $+x$) propagation. Parallels are drawn both to the one-dimensional limit of this problem (waves on an inhomogeneous string [1, 2]), in which this splitting technique produces uncoupled ordinary differential equations (ODEs), and also to other more complex “virtually” one-dimensional cases (e.g., in acoustics and elasticity [3, 4]), in which the decoupled fields propagate via a hierarchy of parabolic partial differential equations (PDEs) of similar form to those obtained here.

It will be shown that after the m^{th} transformation, the Helmholtz equation assumes the form

$$\frac{\partial}{\partial x} \begin{pmatrix} \ell^{(m)} \\ r^{(m)} \end{pmatrix} = \underbrace{\begin{pmatrix} a^{(m)} + d^{(m)} & b^{(m)} - ic^{(m)} \\ b^{(m)} + ic^{(m)} & a^{(m)} - d^{(m)} \end{pmatrix}}_{G^{(m)}} \begin{pmatrix} \ell^{(m)} \\ r^{(m)} \end{pmatrix} + O(\varepsilon^{m+1}), \quad (1)$$

the $a^{(m)}, \dots, d^{(m)}$ terms of which contain a transverse differential operator ε that is assumed to be small in a specified sense. When the generator matrix $G^{(m)}$ is required, through m^{th} order, to be *diagonal* ($b^{(m)} = c^{(m)} = 0$ so that $\ell^{(m)}$ and $r^{(m)}$ are decoupled) as well as *balanced* ($a^{(m)} = 0$) and *symmetrized* ($d^{(m)}$ has the necessary symmetry so that left-right inversion of the problem simply swaps $\ell^{(m)}$ and $r^{(m)}$), this splits the Helmholtz field into left- and right-going components that obey $\partial \ell^{(m)} / \partial x = d^{(m)} \ell^{(m)}$ and $\partial r^{(m)} / \partial x = -d^{(m)} r^{(m)}$, respectively. Owing to the pseudounitariness of the transformations, the original energy is conserved at each order, m and the two counterpropagating components separately transport their shares of the total. The form of $d^{(m)}$ that accomplishes this splitting is shown to be unique. Through order $m = 2$, $d^{(m)}$ contains nothing but the m leading terms of the formal Taylor series for $-i\sqrt{1 + 2\varepsilon}$, with $d^{(1)}$ being the “standard” PE operator [5]. Beginning at $m = 3$, however, a phenomenon originally noted

by Wurmser et al. [4] appears: $d^{(m)}$ acquires additional m^{th} -order, non-Taylor-series terms involving x derivatives of the refractive index.

2. BACKGROUND

This section presents background information about the membrane concerning the dynamics in general, its state-space description, and ducted propagation.

2.1 Membrane Dynamics

At rest, the membrane occupies the $\vec{r} = (x, y)$ plane at $z = 0$. In the linear-response regime, any z displacement $w(\vec{r}, t)$ evolves according to the 2-D wave equation^a

$$\rho \partial_t^2 w - \tau (\partial_{\vec{r}} \cdot \partial_{\vec{r}}) w = 0, \quad (2)$$

with phase speed $c = \sqrt{\tau/\rho}$, in which τ and ρ are the surface tension and mass density. In our case, τ will be a constant but ρ may depend continuously^b on \vec{r} . Energy conservation is embodied in $\partial_{\vec{r}} \cdot \vec{p} + \partial_t e = 0$, in which $e = \frac{1}{2} \rho (\partial_t w)^2 + \frac{1}{2} \tau (\partial_{\vec{r}} w)^2$ is the energy density and $\vec{p} = -\tau (\partial_t w) (\partial_{\vec{r}} w)$ is the energy flux.

For the cw case, with $w(\vec{r}, t) = a(\vec{r}) e^{-i\omega t}$, the complex amplitude obeys the 2-D Helmholtz equation

$$(\partial_{\vec{r}} \cdot \partial_{\vec{r}} + k^2) a = 0, \quad (3)$$

whose wave number $k = \omega/c$ is, in general, a function of \vec{r} . Energy conservation reduces to $\partial_{\vec{r}} \cdot \vec{p} = 0$, in which

$$\vec{p} = -\frac{i\omega\tau}{4} (a^* \partial_{\vec{r}} a - a \partial_{\vec{r}} a^*) \quad (4)$$

is now the *time-averaged* energy flux.

We use the membrane's minimum density $\rho_0 = \min(\rho)$ to define the reference values $c_0 = \sqrt{\tau/\rho_0} = \max(c)$, $k_0 = \omega/c_0 = \min(k)$, and $\lambda_0 = 2\pi/k_0 = \max(\lambda)$ in terms of which the refractive index is $n = c_0/c = \lambda_0/\lambda = k/k_0 = \sqrt{\rho/\rho_0} \geq 1$. For convenience, we also define $\epsilon = \frac{1}{2}(n^2 - 1) \geq 0$, a function of x and y that vanishes identically if the membrane is completely uniform. Finally, we rescale \vec{r} to $k_0 \vec{r}$, so that distances are measured out in reference wavelengths; however, for simplicity, we continue to designate this dimensionless position vector “ \vec{r} ”. Thus, Eqs. (3) and (4) become

^a Subscript notation is used for partial derivative operators; e.g., $\partial_{\xi} Q = \partial Q / \partial \xi$.

^b In principle, a density $\rho(x, y)$ that is discontinuous across one or more lines $y = h(x)$ could be handled by the present approach, provided that h varied negligibly with x over the space of a wavelength; however, this would only further complicate the presentation. The proper handling of situations with significant h variability on the wavelength scale is surprisingly tricky [3]. For simplicity, density discontinuities of all types are explicitly avoided here.

$$(\partial_{\vec{r}} \cdot \partial_{\vec{r}} + 1 + 2\epsilon)a = 0 \quad (5)$$

and

$$\vec{p} = -i\alpha(a^* \partial_{\vec{r}} a - a \partial_{\vec{r}} a^*) , \quad (6)$$

in which $\alpha = \rho_0 c_0 (\omega/2)^2$ is a constant. We restrict our consideration to cases in which $\rho(x, y)$ has a pronounced maximum in the vicinity of $y=0$ and tapers off to its global minimum at large $|y|$. Thus, $c(x, y)$ has a minimum near $y=0$, which we assume is strong enough to form a significant duct along the x axis.

2.2 Splitting the Helmholtz Equation

By defining the transverse differential operator

$$\epsilon = \epsilon + \frac{1}{2} \partial_y^2 , \quad (7)$$

one can write Eq. (5) as

$$[\partial_x^2 + (1 + 2\epsilon)]a = 0 . \quad (8)$$

The operator $1 + 2\epsilon$ is simply $n^2(x, y) + \partial_y^2$ so that, despite its altered appearance, this is still just the Helmholtz equation — an elliptic PDE. It has long been recognized [5] that, when the environment has no x dependence at all (i.e., when $n = n(y)$ so that the operators ∂_x^2 and ϵ commute), one can formally factor Eq. (8) into

$$\underbrace{(\partial_x - d)}_{\text{left}} \underbrace{(\partial_x + d)}_{\text{right}} a = 0 , \quad (9)$$

in which [6]

$$d = -i\sqrt{1 + 2\epsilon} \quad (10)$$

(Tappert's Q operator [5]) with some suitable definition for the square root. The left and right factors commute and should both produce solutions. However, it is difficult to know how to extend this insight to x -dependent environments in a way that is both mathematically satisfactory and physically appropriate. Indeed,

The construction, approximation, and understanding of the square-root Helmholtz operator have been major problems in wave propagation and scattering for, at least, the past fifty years in areas as diverse as acoustics, electromagnetics, optics, seismics, and pure, applied, and computational mathematics. [7, p.1637]

The difficulty is related to the fact that d is a pseudodifferential operator [8]. Although considerable progress has been made towards mathematically rigorous results (Ref. 7 and citations therein), especially for particular special cases [9], the general theory is still under development.

Rather than trying to contribute to those mathematical efforts, the present report attempts to shed some light on the matter through another approach, namely, adapting the technique of Foldy-Wouthuysen transformations, which has proven useful in a similar context in the quantum physics of atomic and subatomic systems. In the interest of clarity, two points should be stressed at the outset. Firstly, this is a method from mathematical physics that is, so to speak, more physics than mathematics. To the best of the author's knowledge, there has never been a thoroughgoing mathematical critique of the technique. Its standing among physicists derives from its demonstrated capacity to generate results in agreement with experiment and its success at predicting effects that were subsequently confirmed in the laboratory. Secondly, though the technique arose in the world of quantum physics and is often described using the vocabulary of that field, there is actually nothing quantum mechanical about it at all. It is simply a physically motivated technique for splitting an elliptical equation into a pair of uncoupled PEs under certain conditions.

The starting point is the familiar observation [5] that, for small ε , the formal Taylor series $\sqrt{1+2\varepsilon} = 1 + \varepsilon - \varepsilon^2/2 + \dots$ yields physically reasonable results. In an x -independent environment, when this series is truncated at 1st order, the left and right factors $(\partial_x \mp d)a = 0$ reduce to $(\partial_x \pm i(1 + \epsilon + \frac{1}{2}\partial_y^2))a = 0$. With $a = \ell = e^{-ix}L$ and $a = r = e^{+ix}R$, respectively, these become

$$\begin{aligned}\frac{\partial}{\partial x}L &= -i\left(\epsilon + \frac{1}{2}\frac{\partial^2}{\partial y^2}\right)L \\ \frac{\partial}{\partial x}R &= +i\left(\epsilon + \frac{1}{2}\frac{\partial^2}{\partial y^2}\right)R,\end{aligned}\tag{11}$$

the “standard” PE formulation for propagation to the left and right. Since L and R are slowly varying modulations, this outcome is widely held to be valid to lowest order even for cases in which ϵ has a gradual x dependence. It seems intuitively reasonable that retaining more terms in the Taylor series might produce a similar but more accurate result. Indeed, this is what happens, up to a point. However, it turns out that if energy is to be scrupulously conserved, additional non-Taylor-series terms must be included beginning at the third order. The Foldy-Wouthuysen approach followed below is a means of generating these necessary departures from the $\sqrt{1+2\varepsilon}$ Taylor series for environments in which the x dependence is gradual in a specific sense.

2.3 State-Space Description

2.3.1 Initial Representation

In terms of the 2×1 “state vector”

$$\underline{u} = \begin{pmatrix} a \\ \dot{a} \end{pmatrix},\tag{12}$$

composed of the membrane's vertical displacement a and its longitudinal slope $\dot{a} = \partial a / \partial x$, the 2-D Helmholtz equation (Eq. (5)) assumes the form

$$\partial_x \underline{u} = \underline{G} \underline{u},\tag{13}$$

featuring the 2×2 “generator” matrix

$$\underline{G} = \begin{pmatrix} 0 & 1 \\ -(1+\varepsilon) & 0 \end{pmatrix} = -\varepsilon\sigma_1 + i(1+\varepsilon)\sigma_2. \quad (14)$$

The second form expresses \underline{G} in terms of the Pauli matrices (Ref. 10, Ch. XIII, Sec. 9),

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (15)$$

with the unit matrix σ_0 included.

The dynamics of the membrane have been expressed in terms of the 2×1 “state vector” (Eq. (12)) and the 2×2 “generator” matrix (Eq. (14)). Beneath the superficial resemblance to the string problem [1, 2] lies a crucial difference: \underline{G} depends on the *transverse* coordinate y as well as the longitudinal coordinate x , and the ordinary function ε has been replaced by the transverse differential operator ε . Although the quotes will be dropped hereafter, this distinction should be kept in mind.

The analysis could begin at this point; however, since the eventual solution will emerge from a perturbation process that relies on ε being “small” in some sense, it will be simpler first to shift to a representation in which the generator matrix becomes diagonal whenever ε vanishes. This is accomplished through the transformation $Uu = \underline{u}$, in which

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}, \quad (16)$$

is a unitary matrix.

2.3.2 d’Alembert Representation

In this new “d’Alembert” representation, the state vector is

$$u = \frac{1}{\sqrt{2}} \begin{pmatrix} a + i\dot{a} \\ a - i\dot{a} \end{pmatrix} \equiv \begin{pmatrix} \ell \\ r \end{pmatrix}, \quad (17)$$

and the Helmholtz equation retains the canonical form

$$\partial_x u = Gu \quad (18)$$

in terms of the transformed generator

$$G = \begin{pmatrix} -i(1+\varepsilon) & -i\varepsilon \\ i\varepsilon & i(1+\varepsilon) \end{pmatrix} = -i(1+\varepsilon)\sigma_3 + \varepsilon\sigma_2. \quad (19)$$

The longitudinal and transverse components of the energy flux \vec{p} are

$$p_x = \alpha u^\dagger P_\parallel u \quad (20)$$

and

$$p_y = \alpha u^\dagger P_\perp u, \quad (21)$$

in which the \dagger superscript indicates a complex-conjugated matrix transpose, i.e., $u^\dagger = (\ell^*, r^*)$, and P_\parallel and P_\perp are the 2×2 matrix operators

$$P_\parallel = -\sigma_3 \quad (22)$$

and

$$P_\perp = i(\partial_y^\dagger - \partial_y) \frac{1}{2}(\sigma_0 + \sigma_1). \quad (23)$$

The \dagger superscript in Eq. (23) has a different meaning that will be addressed later. In fact, ∂_y^\dagger is a transverse derivative operator that acts to the *left*; i.e., $v\partial_y^\dagger = \partial_y v$.

Superficially, Eq. (18) resembles a state-space formulation [11]; however, it is a PDE. For a genuine state-space description, it would have to be replaced by an ODE. That is exactly what happens when the problem is reduced to the “string” limit [1, 2]: the transverse (y) coordinate disappears from the picture, and the state vector evolves via an ODE that is simply Eq. (18) with the operator $\varepsilon = \varepsilon(x, y) + \frac{1}{2}\partial_y^2$ replaced by the function $\varepsilon(x)$. Then, $G = -i(1 + \varepsilon(x))\sigma_3 + \varepsilon(x)\sigma_2$, is an ordinary numerical-valued generator matrix, and a well-defined propagator governs the system’s evolution^c in either direction along the x axis from any initial point x_0 . For the membrane, however, such a simple result is not really achievable in any exact sense because the evolution equation always remains an elliptic PDE in x and y . A state-space description for the membrane can only apply in an approximate sense and only in environments in which there is no backscatter (or at most a kind of “virtual” backscatter [3]). In the present work the original Helmholtz equation which, being an elliptic PDE, does not lend itself to solution by numerical marching methods, is “split” into a pair of parabolic PDEs to which marching methods can readily be applied. Naturally, this splitting cannot be achieved exactly. How to do it in a systematic, physically motivated way is the crux of the matter.

2.3.3 Asymptotic Ducted Propagation

For the membrane problem, we will be especially concerned with the total *longitudinal* energy flux,

$$p_\parallel(x) = \int_{-\infty}^{\infty} p_x(x, y) dy. \quad (24)$$

In Dirac’s bra/ket notation (Ref. 1, Ch. 1, Sec. 6), this can be written as

$$p_\parallel(x) = \alpha \langle u(x, \cdot) | P_\parallel | u(x, \cdot) \rangle, \quad (25)$$

in terms of the inner product

$$\langle u(x, \cdot) | v(x, \cdot) \rangle = \int_{-\infty}^{\infty} u^\dagger(x, y) v(x, y) dy, \quad (26)$$

^c When ε vanishes identically for the string case, Eq. (17) supports solutions consisting of two waveforms (the d’Alembert modes) that propagate without distortion in the $+x$ and $-x$ senses. This makes it a useful representation in which to begin analyzing the membrane when ε is only weakly x dependent.

which involves both matrix multiplication and transverse integration. The operator ∂_y^\dagger , as the notation suggests, is the adjoint of ∂_y relative to this inner product. The state vector $|u(x, y)\rangle$ satisfies $\partial_x |u\rangle = G |u\rangle$. Its dual-space adjoint $\langle u(x, y)|$ satisfies $\partial_x \langle u| = \langle u| G^\dagger$ in terms of the adjoint operator $G^\dagger = +i(1 + \varepsilon^\dagger)\sigma_3 + \varepsilon^\dagger\sigma_2$, where $\varepsilon^\dagger = \varepsilon + \frac{1}{2}\partial_y^2$. Note that $\partial_y^\dagger = -\partial_y$ so that $(\partial_y^2)^\dagger = \partial_y^2$. Consequently, ε is Hermitian: $\varepsilon = \varepsilon^\dagger$. The operators representing the energy flux components are also Hermitian ($P_\parallel^\dagger = P_\parallel$ and $P_\perp^\dagger = P_\perp$).

Integrating Eq. (25) by parts yields

$$\partial_x P_\parallel(x) = \alpha \int_{-\infty}^{\infty} u^\dagger(x, y) \frac{i}{2} (\sigma_0 + \sigma_1) u(x, y) dy = -\alpha u^\dagger(x, y) P_\perp u(x, y) \Big|_{y=-\infty}^{y=\infty} = -p_y(x, y) \Big|_{y=-\infty}^{y=\infty}, \quad (27)$$

which is a statement about energy conservation: any energy not flowing longitudinally along the duct must be leaking away in the transverse direction. We will restrict consideration to ducted fields — those that propagate paraxially without any leakage.

3. FURTHER TRANSFORMATIONS

The essence of the present method is to apply a series of transformations that progressively diagonalizes the generator while strictly conserving the longitudinal energy flux. In Section 3.1, such transformations are considered for a general x -dependent environment. In Section 3.2, the analytic form is given for an x -independent environment.

3.1 General Environment

The state-space description is analogous^d to the evolution of a two-state quantum system via the Schrödinger equation, $i\partial_t |u\rangle = H |u\rangle$ (in units for which $\hbar = 1$). The analog Hamiltonian is $H = iG$ and x plays the role of time. One may define the “matrix element” $\varphi(x) = \langle u(x, \cdot) | \Phi(x, \cdot) | u(x, \cdot) \rangle$ for an arbitrary operator $\Phi(x, y)$. Then φ obeys

$$\partial_x \varphi = \langle u | G^\dagger \Phi + \Phi G + \dot{\Phi} | u \rangle, \quad (28)$$

in which, as always, the dot denotes a longitudinal derivative, $\dot{\xi} = \partial \xi / \partial x$. In general, in order for φ to be independent of x we would need to have $G^\dagger \Phi + \Phi G + \dot{\Phi} = 0$. When the operator Φ lacks any intrinsic x dependence, i.e., when $\dot{\Phi} = 0$, that condition reduces to $G^\dagger \Phi + \Phi G = 0$; i.e., to $H^\dagger \Phi = \Phi H$. Any such invariant is a constant of the motion. (Per quantum-mechanical usage, this term is applied to both φ and Φ .) In quantum mechanical problems, this always applies to the unit operator $\Phi = \sigma_0$ so that the Hamiltonian is Hermitian ($H^\dagger = H$) and the normalization of the wave function is thus preserved ($\varphi = \|u\|^2 = \text{constant}$) during the system’s evolution in time. Any transformation $M |\tilde{u}\rangle = |u\rangle$ to another representation is allowed, provided it is unitary, i.e., $M^\dagger = M^{-1}$ so that the Hamiltonian remains Hermitian after the transformation $\tilde{H}^\dagger = \tilde{H}$.

^d The analogy is to the wave motion itself, *not* to any quantum phenomena.

For the membrane dynamics, the constant of the motion is instead $\Phi = P_{\parallel}$ and the Hamiltonian is consequently *pseudo-Hermitian* [4]: $H^{\dagger}P_{\parallel} = P_{\parallel}H$. (Note that Eq. (27) explicitly restricts the pseudo-Hermiticity of H to *ducted* fields.) Any linear transformation $M|\tilde{u}\rangle = |u\rangle$ is allowed provided it is *pseudo-unitary*, $M^{\dagger}P_{\parallel} = P_{\parallel}M^{-1}$, to ensure that p_{\parallel} retains its status as constant of the motion in the new representation. The transformed equation and longitudinal energy flux are

$$\partial_x |\tilde{u}\rangle = \tilde{G} |\tilde{u}\rangle \quad (29)$$

and

$$p_{\parallel} = \alpha \langle \tilde{u} | \tilde{P}_{\parallel} | \tilde{u} \rangle , \quad (30)$$

in terms of the transformed operators and

$$\tilde{P}_{\parallel} = M^{\dagger} P_{\parallel} M \quad (31)$$

and

$$\tilde{G} = \tilde{A} + \tilde{R} , \quad (32)$$

in which

$$\tilde{A} = M^{-1} G M \quad (33)$$

and

$$\tilde{R} = -M^{-1} \dot{M} . \quad (34)$$

Without any loss of generality, we adopt the exponential form $M = e^{-B}$, which is pseudounitary whenever iB is pseudo-Hermitian; i.e., whenever

$$B^{\dagger} \sigma_3 + \sigma_3 B = 0 . \quad (35)$$

We proceed by seeking a form for B that will produce a diagonal \tilde{G} .

3.2 Longitudinally Invariant Environment

It is well known that when the environment is independent of x , this diagonalization can be done exactly [3]. The correct general form (produced by $B = \frac{1}{2}\psi\sigma_1$) is

$$M = \cosh(\tfrac{1}{2}\psi)\sigma_0 - \sinh(\tfrac{1}{2}\psi)\sigma_1 = \begin{pmatrix} \cosh(\tfrac{1}{2}\psi) & -\sinh(\tfrac{1}{2}\psi) \\ -\sinh(\tfrac{1}{2}\psi) & \cosh(\tfrac{1}{2}\psi) \end{pmatrix} , \quad (36)$$

in which the parameter ψ does not depend on x . For arbitrary ψ , (a) M is independent of x so that \tilde{R} vanishes and the transformed generator is simply $\tilde{G} = \tilde{A}$, and (b) the back-transformation to the initial representation, $|\underline{u}\rangle = UM|\tilde{u}\rangle$, is given by

$$UM = \frac{1}{\sqrt{2}} \begin{pmatrix} \exp(-\frac{1}{2}\psi) & \exp(-\frac{1}{2}\psi) \\ -i \exp(\frac{1}{2}\psi) & i \exp(\frac{1}{2}\psi) \end{pmatrix}. \quad (37)$$

For the particular value,

$$\psi = \operatorname{arctanh}\left(\frac{\varepsilon}{1+\varepsilon}\right), \quad (38)$$

Eq. (36) produces the diagonal generator,

$$\tilde{G} = \begin{pmatrix} d & 0 \\ 0 & -d \end{pmatrix} = d\sigma_3, \quad (39)$$

in which $d = -i\sqrt{1+2\varepsilon}$. Since $\operatorname{arctanh}\left(\frac{\varepsilon}{1+\varepsilon}\right) = \frac{1}{2}\log(1+2\varepsilon)$, this also results in

$$UM = \frac{1}{\sqrt{2}} \begin{pmatrix} (1+2\varepsilon)^{-\frac{1}{4}} & (1+2\varepsilon)^{-\frac{1}{4}} \\ -i(1+2\varepsilon)^{\frac{1}{4}} & i(1+2\varepsilon)^{\frac{1}{4}} \end{pmatrix}, \quad (40)$$

which leads directly to a membrane z -displacement of the form $a = \frac{1}{\sqrt{2}}(1+2\varepsilon)^{-\frac{1}{4}}(\tilde{\ell} + \tilde{r})$. When only one of the two modes is present — either $\tilde{\ell}$ or \tilde{r} alone — its amplitude is related to a by the WKB factor $\frac{1}{\sqrt{2}}(1+2\varepsilon)^{-\frac{1}{4}}$.

Although this diagonalization can no longer be done exactly when the environment is x -dependent, it can still be done approximately if that dependence is “weak” in the specific sense that $\partial^n \varepsilon / \partial x^n \sim O(\varepsilon^{n+1})$. During this process it is essential to remember that although the operator ε certainly commutes with any expression of the form $f(\varepsilon)$, it does *not* generally commute with other operators — notably its own longitudinal derivative, $\dot{\varepsilon} = \partial \varepsilon / \partial x$. Some preliminary results will be obtained in the following section.

4. MATRIX REPRESENTATIONS

In Section 5, a series of pseudounitary transformations of the form $M = e^{-B}$ will be devised to progressively modify the generator $\tilde{G} = \tilde{A} + \tilde{R}$ by preserving the diagonality of the \tilde{A} term while progressively reducing the size of the nondiagonal term \tilde{R} . The effects of these transformations are formulated in terms of the *commutator* $[B]$, which is defined by $[B]\Phi \equiv [B, \Phi] = B\Phi - \Phi B$ for any operator Φ . The whole development is based on the properties of a particular matrix representation for $[B]$. That representation is introduced here in Section 4, with particular emphasis on two important situations. Cases in which the $[B]$ representation is block-diagonal are discussed in Section 4.1; block off-diagonal cases are treated in Section 4.2.

With $M = e^{-B}$, Eq. (33) becomes

$$\tilde{A} = e^{[B]}G, \quad (41)$$

in which the exponential corresponds to the usual series

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!} = 1 + z + \frac{1}{2}z^2 + \cdots, \quad (42)$$

and Eq. (34) takes the form

$$\tilde{R} = E([B])\dot{B}, \quad (43)$$

in which $E(z) = (e^z - 1)/z$; i.e.,

$$E(z) = \sum_{n=1}^{\infty} \frac{z^{n-1}}{n!} = 1 + \frac{1}{2}z + \frac{1}{6}z^2 + \cdots. \quad (44)$$

Although Eq. (41) is well known (Ref. 14, Ch. 3), Eq. (43) appears to be an original result. (The series in Eq. (44) was not obtained by analytical proof. It was postulated by induction from the first few terms and then verified for the first 100 terms using the MapleTM symbolic computation environment to handle the noncommutative algebra.)

Expressing \tilde{A} and \tilde{R} in the forms shown in Eqs. (41) and (43) suggests that it could be productive to treat state-space operators such as G , \dot{B} , \tilde{A} , and \tilde{R} as vectors in a larger “superspace” and to recast objects like $[B]$ in the role of operators on that space. We will call such entities “supervectors” and “superoperators,” respectively. (This parallels the usage in statistical mechanics, where the terms are applied, respectively, to the density operator and the Liouvillian in the Liouville equation [13].) Since any state-space operator can be represented uniquely by a linear combination of the Pauli matrices, a convenient matrix representation for its supervector manifestation can be had by simply stacking its Pauli coefficients in a column matrix. For example, state-space operators of the forms

$$\begin{aligned} G &= a\sigma_0 + b\sigma_1 + c\sigma_2 + d\sigma_3 \\ B &= p\sigma_0 + q\sigma_1 + r\sigma_2 + s\sigma_3 \end{aligned} \quad (45)$$

(whose a, \dots, d and p, \dots, s coefficients may involve transverse differential operators) can be represented as supervectors by

$$G = \begin{pmatrix} a \\ d \\ b \\ c \end{pmatrix}, \quad B = \begin{pmatrix} p \\ s \\ q \\ r \end{pmatrix}. \quad (46)$$

The entries in the columns are arranged so that those associated with the diagonal Pauli matrices (σ_0 , σ_3) and those associated with the off-diagonal ones (σ_1 , σ_2) are grouped separately. (They are separated by dotted lines in Eqs. (46) and (47).) Corresponding to this representation for the supervector B , the matrix representing the superoperator $[B]$ is

$$[B] = \left(\begin{array}{cc|cc} [p] & [s] & [q] & [r] \\ [s] & [p] & -i\{r\} & i\{q\} \\ \hline [q] & i\{r\} & [p] & -i\{s\} \\ [r] & -i\{q\} & i\{s\} & [p] \end{array} \right), \quad (47)$$

in which the $\{\cdot\}$ notation indicates an *anticommutator*: $\{W\}\Phi \equiv \{W, \Phi\} = W\Phi + \Phi W$. (The notation is a standard one in quantum optics [14].)

The supervector representations shown in Eq. (46) for G and B can be written somewhat more compactly as

$$G = \begin{pmatrix} D \\ N \end{pmatrix}, \quad B = \begin{pmatrix} P \\ Q \end{pmatrix}, \quad (48)$$

in terms of separate “diagonal” (0, 3) and “nondiagonal” (1, 2) submatrices

$$\begin{aligned} D &= \begin{pmatrix} a \\ d \end{pmatrix}, & P &= \begin{pmatrix} p \\ s \end{pmatrix} \\ N &= \begin{pmatrix} b \\ c \end{pmatrix}, & Q &= \begin{pmatrix} q \\ r \end{pmatrix}. \end{aligned} \quad (49)$$

This can also be done with the superoperator representation in Eq. (47):

$$[B] = \begin{pmatrix} \gamma & \alpha \\ \beta & \delta \end{pmatrix}, \quad (50)$$

in which

$$\begin{aligned} \gamma &= \begin{pmatrix} [p] & [s] \\ [s] & [p] \end{pmatrix}, & \alpha &= \begin{pmatrix} [q] & [r] \\ -i\{r\} & i\{q\} \end{pmatrix} \\ \beta &= \begin{pmatrix} [q] & i\{r\} \\ [r] & -i\{q\} \end{pmatrix}, & \delta &= \begin{pmatrix} [p] & -i\{s\} \\ i\{s\} & [p] \end{pmatrix}. \end{aligned} \quad (51)$$

Since α, \dots, δ are 2×2 matrices, they could also be written as linear combinations of the four Pauli matrices. The “diagonal” ones in particular are simply

$$\begin{aligned} \gamma &= \sigma_0[p] + \sigma_1[s] \\ \delta &= \sigma_0[p] + \sigma_2[s]. \end{aligned} \quad (52)$$

Thus far, we have allowed B to have a general form. As noted, however, Eq. (35) must be imposed as a restriction to guarantee the pseudounitariness of e^{-B} . In terms of the p, \dots, s coefficients in Eq. (45), this pseudounitariness condition reduces to a requirement for q and r to be Hermitian and p and s anti-Hermitian; i.e.,

$$p^\dagger = -p, \quad s^\dagger = -s \quad (53)$$

and

$$q^\dagger = q, \quad r^\dagger = r. \quad (54)$$

In the remainder of this section, two special cases are treated. In the first one, the matrix representation for $[B]$ is block-diagonal (i.e., α and β vanish). In the other, it is block off-diagonal (i.e., γ and δ vanish). In both of them, it will be convenient to take $p = 0$ (hence, $P = s|-\rangle$ where $|-\rangle = (0, 1)^T$) so that we always have $\gamma = \sigma_1[s]$ and $\delta = \sigma_2[s]$.

4.1 Block-Diagonal $[B]$

In order to produce a block-diagonal representation for $[B]$, let $q = 0$ and $r = 0$, so that both α and β vanish:

$$[B] = \begin{pmatrix} \gamma & 0 \\ 0 & \delta \end{pmatrix}.$$

As a result,

$$f([B]) = \begin{pmatrix} f(\gamma) & 0 \\ 0 & f(\delta) \end{pmatrix}, \quad (55)$$

for any analytic function f . From the simple forms $\gamma = \sigma_1[s]$ and $\delta = \sigma_2\{s\}$, then^e,

$$\begin{aligned} \gamma^m &= \sigma_0[s]^m & \text{and} & & \delta^m &= \sigma_0\{s\}^m & \text{for even } m \\ \gamma^m &= \sigma_1[s]^m & \text{and} & & \delta^m &= \sigma_2\{s\}^m & \text{for odd } m \end{aligned} \quad (56)$$

Thus, by separating the even and odd powers of z , via $f(z) = f_{\text{even}}(z) + f_{\text{odd}}(z)$, one has

$$f([B]) = \begin{pmatrix} \sigma_0 f_{\text{even}}([s]) + \sigma_1 f_{\text{odd}}([s]) & 0 \\ 0 & \sigma_0 f_{\text{even}}(\{s\}) + \sigma_2 f_{\text{odd}}(\{s\}) \end{pmatrix}. \quad (57)$$

In particular, for the function $\exp(z)$ in Eq. (41), we have $\exp_{\text{even}}(z) = \cosh(z)$ and $\exp_{\text{odd}}(z) = \sinh(z)$, so that

$$\exp([B]) = \begin{pmatrix} \sigma_0 \cosh([s]) + \sigma_1 \sinh([s]) & 0 \\ 0 & \sigma_0 \cosh(\{s\}) + \sigma_2 \sinh(\{s\}) \end{pmatrix} \quad (58)$$

and for the function $E(z)$ in Eq. (43), we have $E_{\text{even}}(z) = \sinh(z)/z \equiv C(z)$ and $E_{\text{odd}}(z) = (\cosh(z) - 1)/z \equiv S(z)$, so that

$$E([B]) = \begin{pmatrix} \sigma_0 C([s]) + \sigma_1 S([s]) & 0 \\ 0 & \sigma_0 C(\{s\}) + \sigma_2 S(\{s\}) \end{pmatrix}. \quad (59)$$

Further, in terms of

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (60)$$

the diagonal and off-diagonal blocks of the B supervector in Eq. (48) are, respectively, $P = |-\rangle_s$ and $Q = |0\rangle$, so that

^e This follows from the Pauli matrices' idempotent property $\sigma_j^2 = \sigma_0$; i.e., from the fact that they are all square roots of the identity matrix σ_0 .

$$\dot{B} = \begin{pmatrix} |-\rangle \dot{s} \\ |0\rangle \end{pmatrix}. \quad (61)$$

Consequently, the diagonal and off-diagonal blocks of the transformed generator

$$\tilde{G} = \begin{pmatrix} \tilde{D} \\ \tilde{N} \end{pmatrix}$$

are

$$\tilde{D} = (\sigma_0 \cosh([s]) + \sigma_1 \sinh([s]))D + (|-\rangle C([s]) + |+\rangle S([s]))\dot{s} \quad (62)$$

and

$$\tilde{N} = (\sigma_0 \cosh(\{s\}) + \sigma_2 \sinh(\{s\}))N. \quad (63)$$

The only surviving requirement for pseudounitariness is $s = -s^\dagger$.

4.2 Block Off-Diagonal [B]

To produce a block off-diagonal [B] representation, let $s = 0$ instead. Since we already have $p = 0$, that means that γ and δ vanish, leaving

$$[B] = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix}, \quad (64)$$

as well as $P = |0\rangle$ and $Q = q|+\rangle + r|-\rangle$. Thus, the surviving pseudounitariness condition is as shown in Eq. (54). Though this case is more complicated than the block-diagonal one, the block off-diagonal nature of [B] is enough to reduce the diagonal and nondiagonal parts of \tilde{G} to

$$\tilde{D} = \sum_{n=0}^{\infty} \frac{(\alpha\beta)^n}{(2n)!} \left(D + \frac{\alpha}{2n+1} \left(N + \frac{\dot{Q}}{2n+2} \right) \right) \quad (65)$$

and

$$\tilde{N} = \sum_{n=0}^{\infty} \frac{(\beta\alpha)^n}{(2n)!} \left(N + \frac{1}{2n+1} (\beta D + \dot{Q}) \right). \quad (66)$$

The matrices α, β make these more difficult to deal with than the matrices in Eqs. (62) and (63); however, Eqs. (65) and (66) do prove useful elsewhere in the report.

In the following section, a series of pseudounitary transformations will be applied to the state-space formulation of the problem for a ducting environment. Transformations with block off-diagonal [B] representations will be used to diagonalize the generator. Those with block-diagonal [B] representations will be used, when required, to balance it. Two representational forms have been devised for the generator:

$$\tilde{G} = \underbrace{(\tilde{a}\sigma_0 + \tilde{d}\sigma_3)}_{\text{1st form}} + \underbrace{(\tilde{b}\sigma_1 + \tilde{c}\sigma_2)}_{\text{2nd form}} = \begin{pmatrix} \tilde{D} \\ \tilde{N} \end{pmatrix},$$

the first form corresponding to its role as an operator on state-space, the second to its role as a vector in the superspace. “Diagonalizing” \tilde{G} means making $\tilde{b} = \tilde{c} = 0$ (i.e., $\tilde{N} = |0\rangle$), and “balancing” it means also making $\tilde{a} = 0$ (i.e., $\tilde{D} \propto |-\rangle$). The result of this effort will be a systematic hierarchy of increasingly higher-order PEs.

5. TRANSFORMING THE GENERATOR

In this section, pseudounitary transformations are applied to reexpress the state-space equation, Eq. (18) in a series of physically equivalent representations. These will be indexed by a superscript m , with $Z^{(m)}$ denoting a quantity Z in the m^{th} representation. The fundamental assumption is that $\partial^n \varepsilon / \partial x^n \sim \varepsilon^{n+1}$. Under this assumption, the approximation to $Z^{(m)}$ that contains only contributions through m^{th} order will be denoted $Z^{[m]}$. (Hence, $Z^{(m)} = Z^{[m]} + O(\varepsilon^{m+1})$.) The transformations are designed so that in the m^{th} representation, the m^{th} -order approximate state-space generator, $G^{[m]}$, ends up diagonal and balanced. This splits the m^{th} -order dynamics into a pair of uncoupled PEs for left- and right-going wave propagation along the duct. We will follow this procedure through $m = 4$, laying out the results here and consigning the full details to the appendix.

5.1 Order $m = 0$

The process begins in the d’Alembert representation (Section. 2.3.2), which we denote by $m = 0$. The equation of motion,

$$\partial_x |u^{(0)}\rangle = G^{(0)} |u^{(0)}\rangle, \quad (67)$$

has a generator $G^{(0)}$, whose supervector representation has diagonal and nondiagonal parts $D^{(0)} = -i(1 + \varepsilon)|-\rangle$ and $N^{(0)} = \varepsilon|-\rangle$. Through 0th order, this generator is already diagonal and balanced,

$$\begin{aligned} N^{(0)} &= |0\rangle + O(\varepsilon) \\ iD^{(0)} &= \sqrt{1 + 2\varepsilon}|-\rangle + O(\varepsilon), \end{aligned} \quad (68)$$

so that the 0th-order wave field consists of left- and right-going modes that propagate via a pair of PEs that are coupled only at 1st order,

$$\left. \begin{aligned} \frac{\partial \ell^{(0)}}{\partial x} &= +d^{[0]} \ell^{(0)} \\ \frac{\partial r^{(0)}}{\partial x} &= -d^{[0]} r^{(0)} \end{aligned} \right\} + O(\varepsilon), \quad (69)$$

with

$$id^{[0]} = 1. \quad (70)$$

5.2 Order $m = 1$

Next we attempt to construct a pseudounitary transformation

$$M^{(0)} |u^{(1)}\rangle = |u^{(0)}\rangle, \quad (71)$$

to the Bremmer ($m = 1$) representation [2], in which the equation of motion,

$$\partial_x |u^{(1)}\rangle = G^{(1)} |u^{(1)}\rangle, \quad (72)$$

has a generator $G^{(1)}$, whose 1st-order form $G^{[1]}$ is diagonal and balanced. The exponential form $M^{(0)} = \exp(-B^{(0)})$ is successful at this, provided that the $[B^{(0)}]$ representation is block off-diagonal with $Q^{(0)} \sim \varepsilon$. In summary,

$$\begin{aligned} B^{(0)} &= q^{(0)} \sigma_1 \\ q^{(0)} &= \frac{1}{2} \varepsilon \end{aligned} \quad (73)$$

yields

$$\begin{aligned} N^{(1)} &= |0\rangle + O(\varepsilon^2) \\ iD^{(1)} &= \sqrt{1+2\varepsilon} |-\rangle + O(\varepsilon^2). \end{aligned} \quad (74)$$

Thus the 1st-order wave field consists of left- and right-going modes that propagate via a pair of PEs that are coupled only at 2nd order,

$$\left. \begin{aligned} \frac{\partial \ell^{(1)}}{\partial x} &= +d^{[1]} \ell^{(1)} \\ \frac{\partial r^{(1)}}{\partial x} &= -d^{[1]} r^{(1)} \end{aligned} \right\} + O(\varepsilon^2). \quad (75)$$

The operator on the right-hand side is given by

$$id^{[1]} = 1 + \varepsilon. \quad (76)$$

5.3 Order $m = 2$

We continue the process, trying to construct a pseudounitary transformation

$$M^{(1)} |u^{(2)}\rangle = |u^{(1)}\rangle \quad (77)$$

to an $m = 2$ representation, in which the equation of motion,

$$\partial_x |u^{(2)}\rangle = G^{(2)} |u^{(2)}\rangle, \quad (78)$$

has a generator $G^{(2)}$ that is diagonal and balanced through 2nd order. The usual form $M^{(1)} = \exp(-B^{(1)})$ works again, provided the $[B^{(1)}]$ representation is block off-diagonal and $Q^{(1)} = i\frac{1}{2}\sigma_2 N_{(2)}^{(1)} \sim \varepsilon^2$. In that case,

$$\begin{aligned}
B^{(1)} &= q^{(1)} \sigma_1 + r^{(1)} \sigma_2 \\
q^{(1)} &= -\frac{1}{2} \varepsilon^2 \\
r^{(1)} &= -\frac{1}{4} \dot{\varepsilon}
\end{aligned} \tag{79}$$

produces

$$\begin{aligned}
N^{(2)} &= |0\rangle + O(\varepsilon^3) \\
iD^{(2)} &= \sqrt{1+2\varepsilon} |-\rangle + O(\varepsilon^3),
\end{aligned} \tag{80}$$

so that the 2nd-order wave field consists of left- and right-going modes that propagate via a pair of PEs

$$\left. \begin{aligned} \frac{\partial \ell^{(2)}}{\partial x} &= +d^{[2]} \ell^{(2)} \\ \frac{\partial r^{(2)}}{\partial x} &= -d^{[2]} r^{(2)} \end{aligned} \right\} + O(\varepsilon^3), \tag{81}$$

which are coupled only at 3rd order. The operator is

$$id^{[2]} = 1 + \varepsilon - \frac{1}{2} \varepsilon^2. \tag{82}$$

5.4 Order $m = 3$

We attempt to use the same procedure to construct a pseudounitary transformation

$$M^{(2)} |u^{(3)}\rangle = |u^{(2)}\rangle \tag{83}$$

to an $m = 3$ representation, in which the equation of motion is

$$\partial_x |u^{(3)}\rangle = G^{(3)} |u^{(3)}\rangle \tag{84}$$

and the generator's 3rd-order approximation $G^{[3]}$ is both diagonal and balanced. This time, however, the familiar form $M^{(2)} = \exp(-B^{(2)})$ with the block off-diagonal $[B^{(2)}]$ representation and $Q^{(2)} \sim \varepsilon^3$, i.e.,

$$\begin{aligned}
B^{(2)} &= q^{(2)} \sigma_1 + r^{(2)} \sigma_2 \\
q^{(2)} &= \frac{2}{3} \varepsilon^3 - \frac{1}{8} \ddot{\varepsilon} \\
r^{(2)} &= \frac{3}{8} \{\varepsilon, \dot{\varepsilon}\}
\end{aligned} \tag{85}$$

does not succeed completely. Instead, it produces an intermediate 3rd-order representation $|\hat{u}^{(3)}\rangle = \exp(B^{(2)}) |u^{(2)}\rangle$, in which the equation of motion,

$$\partial_x |\hat{u}^{(3)}\rangle = \hat{G}^{(3)} |\hat{u}^{(3)}\rangle, \tag{86}$$

has a generator $\hat{G}^{(3)}$ that, through 3rd order, is diagonal but *not* balanced:

$$\begin{aligned}\widehat{N}^{(3)} &= |0\rangle + O(\varepsilon^4) \\ i\widehat{D}^{(3)} &= \sqrt{1+2\varepsilon}|- \rangle + \underbrace{i\frac{1}{8}[\varepsilon, \dot{\varepsilon}]|+ \rangle}_{\text{imbalance}} + O(\varepsilon^4) \quad .\end{aligned}\tag{87}$$

Balance can be provided, however, by a second exponential transformation $\exp(-\widehat{B}^{(2)})|u^{(3)}\rangle = |\widehat{u}^{(3)}\rangle$, in which the $[\widehat{B}^{(2)}]$ representation is block-diagonal with $\widehat{P}^{(2)} \sim \varepsilon^2$, i.e.,

$$\begin{aligned}\widehat{B}^{(2)} &= \widehat{s}^{(2)}\sigma_3 \\ \widehat{s}^{(2)} &= i\frac{1}{8}\dot{\varepsilon} \quad .\end{aligned}\tag{88}$$

The result is the anticipated equation of motion with a generator $G^{(3)}$ that has

$$\begin{aligned}N^{(3)} &= |0\rangle + O(\varepsilon^4) \\ iD^{(3)} &= \left(\sqrt{1+2\varepsilon} - \frac{1}{8}\ddot{\varepsilon}\right)|- \rangle + O(\varepsilon^4) \quad .\end{aligned}\tag{89}$$

Since the 3rd-order approximation $G^{[3]}$ is both diagonal and balanced, the 3rd-order wave field consists of left- and right-going modes that propagate via a pair of PEs coupled only at 4th order,

$$\left. \begin{aligned}\frac{\partial \ell^{(3)}}{\partial x} &= +d^{[3]}\ell^{(3)} \\ \frac{\partial r^{(3)}}{\partial x} &= -d^{[3]}r^{(3)}\end{aligned} \right\} + O(\varepsilon^4) \quad .\tag{90}$$

The operator is given by

$$id^{[3]} = 1 + \varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{2}\varepsilon^3 \boxed{-\frac{1}{8}\ddot{\varepsilon}} \quad .\tag{91}$$

Note that $m=3$ is the first order at which $id^{[m]}$ contains a term (boxed) that does *not* originate in the Taylor series for $\sqrt{1+2\varepsilon}$. The overall transformation from the $m=2$ representation is $M^{(2)} = \exp(-\widehat{B}^{(2)})\exp(-B^{(2)})$.

5.5 Order $m=4$

We now attempt to extend the process to 4th order, seeking a pseudounitary transformation,

$$M^{(3)}|u^{(4)}\rangle = |u^{(3)}\rangle, \tag{92}$$

to an $m=4$ representation, in which the equation of motion is

$$\partial_x |u^{(4)}\rangle = G^{(4)} |u^{(4)}\rangle \tag{93}$$

and $G^{[4]}$ is diagonal and balanced. Once again, the exponential form $M^{(3)} = \exp(-B^{(3)})$ with block off-diagonal $[B^{(3)}]$ and $Q^{(3)} \sim \varepsilon^4$, i.e.,

$$\begin{aligned}
B^{(3)} &= q^{(3)}\sigma_1 + r^{(3)}\sigma_2 \\
q^{(3)} &= -\varepsilon^4 + \frac{1}{4}\{\varepsilon, \ddot{\varepsilon}\} + \frac{3}{8}\dot{\varepsilon}^2 \\
r^{(3)} &= -\frac{19}{32}\{\varepsilon^2, \dot{\varepsilon}\} - \frac{11}{16}\varepsilon\dot{\varepsilon}\varepsilon + \frac{1}{16}\ddot{\varepsilon}
\end{aligned} \tag{94}$$

is not completely successful. Instead, it produces an intermediate 4th-order representation $|\widehat{u}^{(4)}\rangle = \exp(B^{(3)})|u^{(3)}\rangle$, in which the equation of motion,

$$\partial_x |\widehat{u}^{(4)}\rangle = \widehat{G}^{(4)} |\widehat{u}^{(4)}\rangle, \tag{95}$$

has a generator $\widehat{G}^{(4)}$ that, through 4th order, is diagonal but *not* balanced:

$$\begin{aligned}
\widehat{N}^{(4)} &= |0\rangle + O(\varepsilon^5) \\
i\widehat{D}^{(4)} &= \left(\sqrt{1+2\varepsilon} - \frac{1}{8}(\ddot{\varepsilon} + \dot{\varepsilon}^2)\right)|-\rangle - \underbrace{i\frac{1}{16}[\varepsilon^2, \dot{\varepsilon}]|+}_{\text{imbalance}} + O(\varepsilon^5).
\end{aligned} \tag{96}$$

However, balance can again be restored by a second transformation $|u^{(4)}\rangle = \exp(\widehat{B}^{(3)})|\widehat{u}^{(4)}\rangle$, in which the $[\widehat{B}^{(3)}]$ representation is block-diagonal and $\widehat{P}^{(3)} \sim \varepsilon^3$, i.e., and

$$\begin{aligned}
\widehat{B}^{(3)} &= \widehat{s}^{(3)}\sigma_3 \\
\widehat{s}^{(3)} &= -i\frac{1}{16}\{\varepsilon, \dot{\varepsilon}\}.
\end{aligned} \tag{97}$$

The result is the anticipated equation of motion with a generator $G^{(4)}$ that has

$$\begin{aligned}
N^{(4)} &= |0\rangle + O(\varepsilon^5) \\
iD^{(4)} &= \left(\sqrt{1+2\varepsilon} - \frac{1}{8}\ddot{\varepsilon} + \frac{1}{4}\dot{\varepsilon}^2 + \frac{3}{16}\{\varepsilon, \ddot{\varepsilon}\}\right)|-\rangle + O(\varepsilon^5).
\end{aligned} \tag{98}$$

Since $G^{[4]}$ is diagonal and balanced, the 4th-order wave field consists of left- and right-going modes that propagate via a pair of PEs coupled only at 5th order,

$$\left. \begin{aligned} \frac{\partial \ell^{(4)}}{\partial x} &= +d^{[4]}\ell^{(4)} \\ \frac{\partial r^{(4)}}{\partial x} &= -d^{[4]}r^{(4)} \end{aligned} \right\} + O(\varepsilon^5). \tag{99}$$

The operator is given by

$$id^{[4]} = 1 + \varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{2}\varepsilon^3 \boxed{-\frac{1}{8}\ddot{\varepsilon}} - \frac{5}{8}\varepsilon^4 + \boxed{\boxed{\frac{1}{4}\dot{\varepsilon}^2 + \frac{3}{16}\{\varepsilon, \ddot{\varepsilon}\}}} . \tag{100}$$

At this order, $id^{[m]}$ has *two* contributions that are not associated with the Taylor series for $\sqrt{1+2\varepsilon}$: the boxed 3rd-order term from $id^{[3]}$ and a new 4th-order contribution (double boxed). Equation (100) agrees with Eq. (51) of Ref. 4 and Eq. (4.12) of Ref. 3. The overall transformation from the $m=3$ representation is $M^{(3)} = \exp(-\widehat{B}^{(3)})\exp(-B^{(3)})$.

6. SUMMARY AND DISCUSSION

Single-frequency “drumhead” vibrations on an infinite membrane have been considered for the situation in which the membrane’s density $\rho(x, y)$ has only a weak dependence on x (the longitudinal coordinate) but a strong enough transverse maximum at $y \approx 0$ to form a duct along the x axis. For this case, strictly energy-conserving transformations $M^{(m)}$ have been devised that convert the Helmholtz equation (in dimensionless scaled x, y coordinates) into the form

$$\frac{\partial}{\partial x} |u^{(m)}\rangle = G^{[m]} |u^{(m)}\rangle + O(\varepsilon^{m+1}) \quad \text{for } 0 \leq m \leq 4, \quad (101)$$

in which the 2×2 generator matrix $G^{[m]}$ — a function of the transverse differential operator $\varepsilon = \epsilon + \frac{1}{2} \partial_y^2$, with $\epsilon(x, y) = \frac{1}{2}(n^2(x, y) - 1) \geq 0$ — is diagonal. To m^{th} order, Eq. (101) decouples into a pair of separate PEs for longitudinal propagation without backscatter in either direction along the duct. The essential assumption is the smallness condition $\partial^m \varepsilon / \partial x^m \sim \varepsilon^{m+1}$.

The m^{th} representation is related to the 0^{th} (d’Alembert) one through $W^{(m)} |u^{(m)}\rangle = |u^{(0)}\rangle$, in which $W^{(m)}$ is the cumulative transformation, $W^{(m)} = M^{(0)} M^{(1)} \dots M^{(m-1)}$. The d’Alembert representation is related to the original representation composed of the membrane’s displacement a and longitudinal slope \dot{a} by $U |u^{(0)}\rangle = |\underline{u}\rangle$, in which U is a constant unitary matrix, as shown in Eq. (16). The state vectors in the original, d’Alembert, and m^{th} representations are: $|\underline{u}\rangle = \begin{pmatrix} a \\ \dot{a} \end{pmatrix}$, $|u^{(0)}\rangle = \begin{pmatrix} \ell^{(0)} \\ r^{(0)} \end{pmatrix}$, and $|u^{(m)}\rangle = \begin{pmatrix} \ell^{(m)} \\ r^{(m)} \end{pmatrix}$.

To obtain the ducted wave field propagating in either direction to order m :

- (1) Specify displacement-and-slope initial values $|\underline{u}(x_0, y)\rangle$ at some longitudinal starting point x_0 .
- (2) Convert these to initial values in the m^{th} representation via

$$(UW^{[m]})^{-1}(x_0, y) |\underline{u}(x_0, y)\rangle = |u^{(m)}(x_0, y)\rangle. \quad (102)$$

- (3) Solve the m^{th} -order equation of motion to the left or right, i.e., either

$$\frac{\partial \ell^{(m)}(x, y)}{\partial x} = +d^{[m]}(x, y) \ell^{(m)}(x, y) \quad \text{for } x < x_0 \quad \text{given } \ell^{(m)}(x_0, y) \quad (103)$$

or

$$\frac{\partial r^{(m)}(x, y)}{\partial x} = -d^{[m]}(x, y) r^{(m)}(x, y) \quad \text{for } x > x_0 \quad \text{given } r^{(m)}(x_0, y). \quad (104)$$

- (4) Return to the original displacement-and-slope representation

$$|\underline{u}(x, y)\rangle = UW^{[m]}(x, y) |u^{(m)}(x, y)\rangle. \quad (105)$$

The correct form of the operator $id^{[m]}$ for $m \leq 4$ is obtained by truncating

$$id = \underbrace{\sqrt{1+2\varepsilon}}_{\text{Taylor}} - \underbrace{\frac{1}{8}\ddot{\varepsilon}}_{\text{3rd}} + \underbrace{\frac{1}{4}\dot{\varepsilon}^2 + \frac{3}{16}\{\varepsilon, \ddot{\varepsilon}\}}_{\text{4th}} + O(\varepsilon^5) \quad (106)$$

at order m . Besides the terms of the formal Taylor expansion for the square root, this contains the additional 3rd- and 4th-order terms that are the principal result of this work. The effects of the x dependence of $\rho(x, y)$ accumulate during step (3), and for accuracy in higher-order propagation over long ranges, the non-Taylor-series terms are necessary.

On the other hand, the effects of the end-point transformations (from the initial representation and back to it in steps 2 and 4) *do not* accumulate. With that being the case, a reasonable approach for computing $UW^{[m]}(x, y)$ is to assume *local* x -invariance at the end points of the propagation; i.e., to calculate it as if $n = n(y)$, as was actually the case in Section 3.2. This simply means using the WKB form Eq. (40) and obtaining $(UW^{[m]})^{-1}(x_0, y)$ and $UW^{[m]}(x, y)$, by truncating the Taylor expansions of

$$\begin{aligned} (UW)^{-1} &= \frac{1}{\sqrt{2}} \begin{pmatrix} (1+2\varepsilon)^{\frac{1}{4}} & i(1+2\varepsilon)^{-\frac{1}{4}} \\ (1+2\varepsilon)^{\frac{1}{4}} & -i(1+2\varepsilon)^{-\frac{1}{4}} \end{pmatrix} \\ UW &= \frac{1}{\sqrt{2}} \begin{pmatrix} (1+2\varepsilon)^{-\frac{1}{4}} & (1+2\varepsilon)^{-\frac{1}{4}} \\ -i(1+2\varepsilon)^{\frac{1}{4}} & i(1+2\varepsilon)^{\frac{1}{4}} \end{pmatrix} \end{aligned} \quad (107)$$

at the appropriate order.

This overall procedure rests on two basic ideas:

- (1) using the Foldy-Wouthuysen method of strictly energy-conserving transformations with the assumption $\partial_x^n \varepsilon \sim \varepsilon^{n+1}$ to obtain the unique form of the m^{th} -order decoupled PEs, and
- (2) taking the environment to be locally longitudinally invariant at the beginning and end of the propagation so as to exploit the WKB form for the endpoint transformations.

The first was conceived by Wurmser et al. [4] who implemented it in an ocean acoustics application involving a nearly range-invariant, ducting environment. The second seems to have originated with the late F. D. Tappert [15, 5] who suggested that propagation in such situations be done by first extracting a WKB factor at the source, then propagating the remaining auxiliary field (the carrier of the down-range energy flux) to the receiver, and finally including the WKB factor for the receiver. The results obtained here agree with corresponding outcomes in Refs. 3 and 4, where such a procedure is followed in different physical contexts.

In general, a numerical algorithm that models the higher-order ($m > 2$) parabolic propagation equation under the assumption that $id^{[m]}$ is simply the truncated Taylor series for $\sqrt{1+2\varepsilon}$, will need reprogramming in order to incorporate the effects of the non-Taylor-series terms in Eq. (106). The exception is order $m=3$, where the first and largest of these terms appears. At this order, Eq. (106) yields $id^{[3]} = (1 + \varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{2}\varepsilon^3) - \frac{1}{8}\ddot{\varepsilon}$. However, since $\partial^n \varepsilon / \partial x^n$ is simply $\partial^n \varepsilon / \partial x^n$, the final term reduces to $-\frac{1}{8}\ddot{\varepsilon}$, which is not a transverse differential operator but an ordinary function of x and y . The 3rd-order operator is thus $id^{[3]} = (1 + \varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{2}\varepsilon^3) - \frac{1}{8}\ddot{\varepsilon}$. Since $\varepsilon = \varepsilon + \frac{1}{2}\partial_y^2$, the same result can be produced from the Taylor-series form $id^{[3]} = 1 + \varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{2}\varepsilon^3$ by making the replacement $\varepsilon \rightarrow \varepsilon - \frac{1}{8}\ddot{\varepsilon}$ (and dropping 4th- and higher-order terms). This can be implemented by simply reusing the Taylor-series numerical algorithm with the actual density $\rho(x, y)$ replaced by $\rho(x, y) - \frac{1}{8}\partial^2 \rho(x, y) / \partial x^2$.

This work has presented a detailed analysis of one-way ducted wave propagation for the specific case of a vibrating membrane. The objective in writing it has not been to satisfy any perceived groundswell of community interest in vibrating membranes (even the author could not deceive himself that far) but rather to present a full account of a widely applicable solution method in an uncluttered context, with no more complexity than absolutely necessary, so that the essentials would stand out vividly. This method is applicable in atmospheric electromagnetics, optics, ocean acoustics, and other wave-motion disciplines, in which very accurate modeling is required for fields that propagate over long ranges through ducts whose range dependence is weak enough that no energy is backscattered.

ACKNOWLEDGMENTS

This work was done under basic research sponsorship from the Office of Naval Research. The author is grateful to Dr. Daniel Wurmser (NRL) for numerous valuable discussions that have been essential to its successful completion.

REFERENCES

1. R.F. Gragg, "One-Way Propagation in Weakly Nonuniform Media," *Wave Motion*. **27**(2), 95–115 (1998).
2. R.F. Gragg, "Systematic Splitting of Wavefields into Unidirectional Modes: Long-Range Asymptotic Methods for Weakly Nonuniform Media," NRL/FR/7144--96-9799, August 1996.
3. D. Wurmser, "A Parabolic Equation for Penetrable Rough Surfaces: Using the Foldy-Wouthuysen Transformation to Buffer Density Jumps," *Ann. Phys.* **311**(1), 53–80 (2004).
4. D. Wurmser, G. J. Orris, and R. Dashen, "Application of the Foldy-Wouthuysen Transformation to the Reduced Wave Equation in Range-Dependent Environments," *J. Acoust. Soc. Am.* **101**(3), 1309–1327 (1997).
5. F.D. Tappert, "The Parabolic Approximation Method," in *Wave Propagation and Underwater Acoustics*, J. B. Keller and J. S. Papadakis, eds. (Springer-Verlag, New York, 1977), Chap. V, pp. 224–287.
6. D. Wurmser, "Using the Foldy-Wouthuysen Transformation to Derive Acoustic Parabolic Equations that Properly "Dress" Discontinuities," NRL/FR/7100--04-10,018, March 2004.
7. L. Fishman, "Applications of Directional Wavefield Decomposition, Phase Space, and Path Integral Methods to Seismic Wave Propagation and Inversion," *Pure and Applied Geophys.* **159**(7-8), 1637–1679 (2002).
8. M.W. Wong, *An Introduction to Pseudo-Differential Operators*, (World Scientific, New Jersey, 1991).
9. L. Fishman, M. V. de Hoop, and M. J. N. van Stralen, "Exact Constructions of Square-Root Helmholtz Operator Symbols: The Focusing Quadratic Profile," *J. Math. Phys.* **41**(7), 4881–4938 (2000).
10. A. Messiah, *Quantum Mechanics*, (Wiley and Sons, New York, 1965).

11. B. Friedland, *Control System Design: An Introduction to State-Space Methods*, (McGraw-Hill, New York, 1986).
12. P.A.M. Dirac, *The Principles of Quantum Mechanics*, 4th Ed., (Oxford University Press, England, 1958).
13. L.E. Reichl, *A Modern Course in Statistical Mechanics*, (University of Texas Press, Austin, 1980).
14. W.H. Louisell, *Quantum Statistical Properties of Radiation*, (Wiley and Sons, New York, 1973).
15. F.D. Tappert, "A Range Refraction Parabolic Equation," *J. Acoust. Soc. Am.* **76**(6), 1797–1803 (1984).

Appendix

DETAILS OF THE TRANSFORMATIONS

A1. INTRODUCTION

In this appendix, details of the derivations of the transformation operators $M^{(m)}$ cited in the body of the article (Eqs. (73), (79), (85), (88), (94), and (97)) are presented. An expanded notation is used. For any quantity Z that can be expressed as $Z = Z_0 + Z_1 + Z_2 + \dots$, with $Z_k \sim \varepsilon^k$, the following type of notation is applied to various portions of the series:

$$Z = \underbrace{Z_0}_{Z_{(0)}} + \underbrace{Z_1 + Z_2 + Z_3}_{Z_{(1 \dots 3)}} + \dots + \underbrace{Z_k + \dots}_{Z_{(k \dots \infty)}} .$$

The subscripts on the terms indicate the ranges of ε -orders that they contain. It should be carefully noted that these order subscripts are “applied last.” For example, the symbol $\dot{\Phi}_{(1)}^{(m)}$ represents $(\dot{\Phi}^{(m)})_{(1)}$, the order- ε term in the series for $\dot{\Phi}^{(m)}$ — *not* $\partial \Phi_{(1)}^{(m)} / \partial x$. Likewise, $Z_{(2)}^2$ means $(Z^2)_{(2)} = Z_0 Z_2 + Z_1^2 + Z_2 Z_0 \sim \varepsilon^2$ — *not* $(Z_{(2)})^2 = Z_2^2 \sim \varepsilon^4$.

For the m^{th} step, the objective is to find a pseudounitary transformation $M^{(m)}$ that will diagonalize and balance the transformed generator $G^{(m)} = D^{(m)} + N^{(m)}$ through order ε^m . In the above notation, this means a transformation that produces $N_{(0 \dots m)}^{(m)} = |0\rangle$ and $D_{(0 \dots m)}^{(m)} \propto |-\rangle$. It will turn out that not only do such transformations exist at each order, but they are actually unique.

Two types of pseudounitary transformations are applied to carry the generator from one representation to the next. With a *block off-diagonal* transformation, \tilde{G} arises from G through Eqs. (65) and (66), which intermix G ’s diagonal and off-diagonal components. With a *block-diagonal* transformation, the connection is provided by Eqs. (62) and (63), which keep diagonal and off-diagonal components separate. The Taylor Series for the four functions that appear in Eqs. (62) and (63) are

$$\begin{aligned} \cosh(z) &= 1 + \frac{1}{2} z^2 + \frac{1}{4!} z^4 + \dots \\ \sinh(z) &= z + \frac{1}{3!} z^3 + \frac{1}{5!} z^5 + \dots \\ C(z) &= 1 + \frac{1}{3!} z^2 + \frac{1}{5!} z^4 + \dots \\ S(z) &= \frac{1}{2} z + \frac{1}{4!} z^3 + \frac{1}{6!} z^5 + \dots \end{aligned}$$

After each transformation, it will be found that the dynamics follow the canonical decoupled form

$$\begin{aligned}\frac{\partial \ell(x, y)}{\partial x} &= -d(x, y)\ell(x, y) \\ \frac{\partial r(x, y)}{\partial x} &= +d(x, y)r(x, y),\end{aligned}$$

to the appropriate order of approximation, in which $d(x, y)$ is the sum of two parts. The first is simply a polynomial function $T(\varepsilon(x, y))$, the truncated formal Taylor series for $\sqrt{1+2\varepsilon(x, y)}$. The second part is the non-Taylor-series terms. Their details emerge from the following paragraphs; however, there is a symmetry-related restriction on their structure that is clear at this point. A typical form for such a non-Taylor-series term is

$$\varepsilon^J(x, y) \left(\frac{\partial^K \varepsilon^L(x, y)}{\partial x^K} \right)^M \varepsilon^N(x, y),$$

in which J, K, L, M, N are nonnegative integers. Thus,

$$\begin{aligned}\frac{\partial \ell(x, y)}{\partial x} &= - \left\{ T(\varepsilon(x, y)) + \underbrace{A \varepsilon^J(x, y) \left(\frac{\partial^K \varepsilon^L(x, y)}{\partial x^K} \right)^M \varepsilon^N(x, y)}_{\text{typical}} \right\} \ell(x, y) \\ \frac{\partial r(x, y)}{\partial x} &= + \{ \text{same} \} r(x, y),\end{aligned}$$

where A is some constant. For simplicity, this includes only a single typical non-Taylor-series term. It would be trivial to extend the present argument to the general case. If the environment is reflected in the longitudinal direction through $\varepsilon(x, y) \mapsto \varepsilon(-x, y)$, this becomes

$$\begin{aligned}\frac{\partial \tilde{\ell}(x, y)}{\partial x} &= - \left\{ T(\varepsilon(-x, y)) + \underbrace{A \varepsilon^J(-x, y) \left(\frac{\partial^K \varepsilon^L(-x, y)}{\partial x^K} \right)^M \varepsilon^N(-x, y)}_{\text{typical}} \right\} \tilde{\ell}(x, y) \\ \frac{\partial \tilde{r}(x, y)}{\partial x} &= + \{ \text{same} \} \tilde{r}(x, y) .\end{aligned}$$

And if the direction of the x axis is reversed ($x \mapsto -x$), this becomes

$$\begin{aligned}\frac{\partial \tilde{\ell}(-x, y)}{\partial x} &= + \left\{ T(\varepsilon(x, y)) + \underbrace{A(-1)^{KM} \varepsilon^J(x, y) \left(\frac{\partial^K \varepsilon^L(x, y)}{\partial x^K} \right)^M \varepsilon^N(x, y)}_{\text{typical}} \right\} \tilde{\ell}(-x, y) \\ \frac{\partial \tilde{r}(-x, y)}{\partial x} &= - \{ \text{same} \} \tilde{r}(-x, y) .\end{aligned}$$

Left-right symmetry demands that $\tilde{\ell}(-x, y) = r(x, y)$ and $\tilde{r}(-x, y) = \ell(x, y)$. For this, the ε exponents J, L, N are immaterial, but it is essential that the product $K \times M$ be an *even* integer. Thus, for example, the non-Taylor-series part might include such terms as $\partial^2 \varepsilon / \partial x^2$, $(\partial \varepsilon / \partial x)^2$, and $\varepsilon \partial^2 \varepsilon / \partial x^2$, in which $K \times M = 2$; however, it could not contain terms like $\partial \varepsilon^2 / \partial x$ or $\partial \varepsilon^3 / \partial x$ because they have $K \times M = 1$.

With this symmetry in mind, we proceed to derive the transformation operators $M^{(m)}$ for $m = 0, 1, 2, 3$.

A2. ORDER $m = 0$

The process begins in the d'Alembert representation as shown in Eq. (19), where the superoperator representation of the generator $G^{(0)}$ is composed of $D^{(0)} = -i(1 + \varepsilon)|-\rangle$ and $N^{(0)} = \varepsilon|-\rangle$. Thus,

$$D^{(0)} = D_{(0)}^{(0)} + D_{(1)}^{(0)} \quad (\text{A.1})$$

and

$$N^{(0)} = N_{(1)}^{(0)}, \quad (\text{A.2})$$

in which

$$\begin{aligned} D_{(0)}^{(0)} &= -i|-\rangle \\ D_{(1)}^{(0)} &= -i\varepsilon|-\rangle \\ N_{(1)}^{(0)} &= \varepsilon|-\rangle. \end{aligned} \quad (\text{A.3})$$

A3. ORDER $m = 1$

For the first step, to the Bremmer representation [1], we look for an operator $Q^{(0)} \sim \varepsilon$ to produce a transformation $Q^{(0)} : G^{(0)} \rightarrow G^{(1)}$ that achieves the desired degree of diagonalization, $N_{(0 \dots 1)}^{(1)} = |0\rangle$. Since $Q^{(0)} = Q_{(1)}^{(0)}$, it follows that $\alpha^{(0)} = \alpha_{(1)}^{(0)}$, $\beta^{(0)} = \beta_{(1)}^{(0)}$, and $\dot{Q}^{(0)} = \dot{Q}_{(2)}^{(0)}$. Thus, Eqs. (65) and (66) with $G = G^{(0)}$ and $\tilde{G} = G^{(1)}$ yield

$$\begin{aligned} D_{(0 \dots 4)}^{(1)} &= D_{(0 \dots 1)}^{(0)} + \alpha_{(1)}^{(0)} \left(N_{(1)}^{(0)} + \frac{1}{2} \dot{Q}_{(2)}^{(0)} \right) \\ &\quad + \frac{1}{2} \alpha_{(1)}^{(0)} \beta_{(1)}^{(0)} \left(D_{(0 \dots 1)}^{(0)} + \frac{1}{3} \alpha_{(1)}^{(0)} N_{(1)}^{(0)} \right) \\ &\quad + \frac{1}{4!} \left(\alpha_{(1)}^{(0)} \beta_{(1)}^{(0)} \right)^2 D_{(0)}^{(0)} \end{aligned} \quad (\text{A.4})$$

and

$$\begin{aligned} N_{(0 \dots 4)}^{(1)} &= N_{(1)}^{(0)} + \beta_{(1)}^{(0)} D_{(0 \dots 1)}^{(0)} + \dot{Q}_{(2)}^{(0)} \\ &\quad + \frac{1}{2} \beta_{(1)}^{(0)} \alpha_{(1)}^{(0)} \left(N_{(1)}^{(0)} + \frac{1}{3} \left(\beta_{(1)}^{(0)} D_{(0 \dots 1)}^{(0)} + \dot{Q}_{(2)}^{(0)} \right) \right). \end{aligned} \quad (\text{A.5})$$

The subscripts facilitate grouping the terms by order:

$$\begin{aligned} D_{(0 \dots 1)}^{(1)} &= D_{(0 \dots 1)}^{(0)} \\ D_{(2)}^{(1)} &= \alpha_{(1)}^{(0)} \left(N_{(1)}^{(0)} + \frac{1}{2} \beta_{(1)}^{(0)} D_{(0)}^{(0)} \right) \\ D_{(3)}^{(1)} &= \frac{1}{2} \alpha_{(1)}^{(0)} \left(\dot{Q}_{(2)}^{(0)} + \beta_{(1)}^{(0)} D_{(1)}^{(0)} \right) \\ D_{(4)}^{(1)} &= \frac{1}{6} \alpha_{(1)}^{(0)} \beta_{(1)}^{(0)} \alpha_{(1)}^{(0)} \left(N_{(1)}^{(0)} + \frac{1}{4} \beta_{(1)}^{(0)} D_{(0)}^{(0)} \right) \end{aligned} \quad (\text{A.6})$$

and

$$\begin{aligned}
N_{(0)}^{(1)} &= |0\rangle \\
N_{(1)}^{(1)} &= N_{(1)}^{(0)} + \beta_{(1)}^{(0)} D_{(0)}^{(0)} \\
N_{(2)}^{(1)} &= \beta_{(1)}^{(0)} D_{(1)}^{(0)} + \dot{Q}_{(2)}^{(0)} \\
N_{(3)}^{(1)} &= \frac{1}{2} \beta_{(1)}^{(0)} \alpha_{(1)}^{(0)} \left(N_{(1)}^{(0)} + \frac{1}{3} \beta_{(1)}^{(0)} D_{(0)}^{(0)} \right) \\
N_{(4)}^{(1)} &= \frac{1}{6} \beta_{(1)}^{(0)} \alpha_{(1)}^{(0)} \left(\beta_{(1)}^{(0)} D_{(1)}^{(0)} + \dot{Q}_{(2)}^{(0)} \right).
\end{aligned} \tag{A.7}$$

The requirement for diagonalization through order ε is that $N_{(1)}^{(1)} = |0\rangle$; i.e.,

$$\begin{pmatrix} 0 \\ \varepsilon \end{pmatrix} + \begin{pmatrix} [q^{(0)}] & i\{r^{(0)}\} \\ [r^{(0)}] & -i\{q^{(0)}\} \end{pmatrix} \begin{pmatrix} 0 \\ -i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{A.8}$$

This is equivalent to $\{q^{(0)}\}1 = \varepsilon$ and $\{r^{(0)}\}1 = 0$. Since $\{\phi\}1 = 2\phi$ for any ϕ , the outcome is simply

$$q^{(0)} = \frac{1}{2} \varepsilon, \quad r^{(0)} = 0. \tag{A.9}$$

Because $\varepsilon = \varepsilon^\dagger$ for ducted fields, the pseudounitariness conditions in Eq. (54) are satisfied at this stage. Thus,

$$Q^{(0)} = \begin{pmatrix} \frac{1}{2} \varepsilon \\ 0 \end{pmatrix} = \frac{1}{2} \varepsilon |+\rangle = \frac{i}{2} \sigma_2 N_{(1)}^{(0)}. \tag{A.10}$$

As a result,

$$\dot{Q}^{(0)} = \begin{pmatrix} \frac{1}{2} \dot{\varepsilon} \\ 0 \end{pmatrix}, \quad \alpha^{(0)} = \begin{pmatrix} \frac{1}{2} [\varepsilon] & 0 \\ 0 & \frac{i}{2} \{\varepsilon\} \end{pmatrix}, \quad \beta^{(0)} = \begin{pmatrix} \frac{1}{2} [\varepsilon] & 0 \\ 0 & -\frac{i}{2} \{\varepsilon\} \end{pmatrix}. \tag{A.11}$$

(This is where $\dot{\varepsilon}$ first appears.) As expected, $\dot{Q}^{(0)} \sim \varepsilon^2$, while $\alpha^{(0)}, \beta^{(0)} \sim \varepsilon$; i.e., $\dot{Q}^{(0)} = \dot{Q}_{(2)}^{(0)}$, $\alpha^{(0)} = \alpha_{(1)}^{(0)}$, and $\beta^{(0)} = \beta_{(1)}^{(0)}$. Equations (A.10) and (A.11) provide matrix representations for Eqs. (A.6) and (A.7). Those terms not already obtained are

$$\begin{aligned}
D_{(2)}^{(1)} &= \begin{pmatrix} 0 \\ \frac{i}{2} \varepsilon^2 \end{pmatrix}, \quad D_{(3)}^{(1)} = \begin{pmatrix} \frac{1}{8} [\varepsilon, \dot{\varepsilon}] \\ -\frac{i}{2} \varepsilon^3 \end{pmatrix}, \quad D_{(4)}^{(1)} = \begin{pmatrix} 0 \\ \frac{i}{8} \varepsilon^4 \end{pmatrix} \\
N_{(2)}^{(1)} &= \begin{pmatrix} \frac{1}{2} \dot{\varepsilon} \\ -\varepsilon^2 \end{pmatrix}, \quad N_{(3)}^{(1)} = \begin{pmatrix} 0 \\ \frac{1}{3} \varepsilon^3 \end{pmatrix}, \quad N_{(4)}^{(1)} = \begin{pmatrix} \frac{1}{48} [\varepsilon, [\varepsilon, \dot{\varepsilon}]] \\ -\frac{1}{6} \varepsilon^4 \end{pmatrix}.
\end{aligned} \tag{A.12}$$

A4. ORDER $m = 2$

For the second step, we look for an operator $Q^{(1)} \sim \varepsilon^2$ to produce a transformation $Q^{(1)} : G^{(1)} \rightarrow G^{(2)}$ that diagonalizes the generator through 2nd order, $N_{(0 \dots 2)}^{(2)} = |0\rangle$. Since $Q^{(1)} = Q_{(2)}^{(1)}$, it follows that $\alpha^{(1)} = \alpha_{(2)}^{(1)}$, $\beta^{(1)} = \beta_{(2)}^{(1)}$, and $\dot{Q}^{(1)} = \dot{Q}_{(3)}^{(1)}$. Thus, Eqs. (65) and (66), with $G = G^{(1)}$ and $\tilde{G} = G^{(2)}$, yield

$$\begin{aligned}
D_{(0 \dots 4)}^{(2)} &= D_{(0 \dots 4)}^{(1)} + \alpha_{(2)}^{(1)} N_{(2)}^{(1)} + \frac{1}{2} \alpha_{(2)}^{(1)} \beta_{(2)}^{(1)} D_{(0)}^{(1)} \\
N_{(0 \dots 4)}^{(2)} &= \beta_{(2)}^{(1)} D_{(0 \dots 2)}^{(1)} + N_{(2 \dots 4)}^{(1)} + \dot{Q}_{(3)}^{(1)}.
\end{aligned} \tag{A.13}$$

Consequently,

$$\begin{aligned} D_{(0\cdots 1)}^{(2)} &= D_{(0\cdots 1)}^{(1)} = D_{(0\cdots 1)}^{(0)} \\ D_{(2\cdots 3)}^{(2)} &= D_{(2\cdots 3)}^{(1)} \\ D_{(4)}^{(2)} &= D_{(4)}^{(1)} + \alpha_{(2)}^{(1)} \left(N_{(2)}^{(1)} + \frac{1}{2} \beta_{(2)}^{(1)} D_{(0)}^{(1)} \right) \end{aligned} \quad (\text{A.14})$$

and

$$\begin{aligned} N_{(0\cdots 1)}^{(2)} &= N_{(0\cdots 1)}^{(1)} = |0\rangle \\ N_{(2)}^{(2)} &= N_{(2)}^{(1)} + \beta_{(2)}^{(1)} D_{(0)}^{(1)} \\ N_{(3)}^{(2)} &= N_{(3)}^{(1)} + \beta_{(2)}^{(1)} D_{(1)}^{(1)} + \dot{Q}_{(3)}^{(1)} \\ N_{(4)}^{(2)} &= N_{(4)}^{(1)} + \beta_{(2)}^{(1)} D_{(2)}^{(1)} \end{aligned} \quad (\text{A.15})$$

The requirement for diagonalization through order ε^2 is that $N_{(2)}^{(2)} = |0\rangle$. In the matrix representation, this means

$$\begin{pmatrix} \frac{1}{2}\dot{\varepsilon} \\ -\varepsilon^2 \end{pmatrix} + \begin{pmatrix} [q^{(1)}] & i\{r^{(1)}\} \\ [r^{(1)}] & -i\{q^{(1)}\} \end{pmatrix} \begin{pmatrix} 0 \\ -i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (\text{A.16})$$

and the solution is

$$q^{(1)} = -\frac{1}{2}\varepsilon^2, \quad r^{(1)} = -\frac{1}{4}\dot{\varepsilon}. \quad (\text{A.17})$$

(Since $\dot{\varepsilon} = \dot{\varepsilon}$ is just an ordinary function, the pseudounitariness conditions are satisfied.) Thus,

$$Q^{(1)} = -\frac{1}{2}\varepsilon^2 |+\rangle - \frac{1}{4}\dot{\varepsilon} |-\rangle = \begin{pmatrix} -\frac{1}{2}\varepsilon^2 \\ -\frac{1}{4}\dot{\varepsilon} \end{pmatrix} = \frac{i}{2}\sigma_2 N_{(2)}^{(1)}. \quad (\text{A.18})$$

Furthermore,

$$\dot{Q}^{(1)} = \begin{pmatrix} -\frac{1}{2}\{\varepsilon, \dot{\varepsilon}\} \\ -\frac{1}{4}\ddot{\varepsilon} \end{pmatrix}, \quad \alpha^{(1)} = \begin{pmatrix} -\frac{1}{2}[\varepsilon^2] & -\frac{1}{4}[\dot{\varepsilon}] \\ \frac{i}{4}\{\dot{\varepsilon}\} & -\frac{i}{2}\{\varepsilon^2\} \end{pmatrix}, \quad \beta^{(1)} = \begin{pmatrix} -\frac{1}{2}[\varepsilon^2] & -\frac{i}{4}\{\dot{\varepsilon}\} \\ -\frac{1}{4}[\dot{\varepsilon}] & \frac{i}{2}\{\varepsilon^2\} \end{pmatrix}. \quad (\text{A.19})$$

Equations (A.18) and (A.19) produce the matrix representatives for the quantities in Eqs. (A.14) and (A.15). Those not already obtained are

$$\begin{aligned} D_{(4)}^{(2)} &= \begin{pmatrix} -\frac{1}{4}[\varepsilon^2, \dot{\varepsilon}] \\ \frac{5i}{8}\varepsilon^4 + \frac{i}{8}\dot{\varepsilon}^2 \end{pmatrix} \\ N_{(3)}^{(2)} &= \begin{pmatrix} -\frac{3}{4}\{\varepsilon, \dot{\varepsilon}\} \\ \frac{4}{3}\varepsilon^3 - \frac{1}{4}\ddot{\varepsilon} \end{pmatrix} \\ N_{(4)}^{(2)} &= \begin{pmatrix} \frac{1}{48}[\varepsilon, [\varepsilon, \dot{\varepsilon}]] + \frac{1}{8}\{\varepsilon^2, \dot{\varepsilon}\} \\ -\frac{2}{3}\varepsilon^4 \end{pmatrix}. \end{aligned} \quad (\text{A.20})$$

A.5 ORDER $m = 3$

For the third step, we look for an operator $Q^{(2)} \sim \varepsilon^3$ to produce a transformation $Q^{(2)} : G^{(2)} \rightarrow \tilde{G}^{(3)}$ that diagonalizes the generator through 3rd order, $\hat{N}_{(0\cdots 3)}^{(3)} = |0\rangle$. Since $Q^{(2)} = Q_{(3)}^{(2)}$, it follows that $\alpha^{(2)} = \alpha_{(3)}^{(2)}$, $\beta^{(2)} = \beta_{(3)}^{(2)}$, and $\dot{Q}^{(2)} = \dot{Q}_{(4)}^{(2)}$. Thus, Eqs. (65) and (66) with $G = G^{(2)}$ and $\tilde{G} = \tilde{G}^{(3)}$ yield

$$\begin{aligned}\hat{D}_{(0\cdots 4)}^{(3)} &= D_{(0\cdots 4)}^{(2)} \\ \hat{N}_{(0\cdots 4)}^{(3)} &= N_{(3\cdots 4)}^{(2)} + \beta_{(3)}^{(2)} D_{(0\cdots 1)}^{(2)} + \dot{Q}_{(4)}^{(2)}.\end{aligned}\tag{A.21}$$

Gathering terms of the same order, one finds that all the “ D ” terms are the same as for $m = 2$ while the “ N ” terms are

$$\begin{aligned}\hat{N}_{(0\cdots 2)}^{(3)} &= N_{(0\cdots 2)}^{(2)} = |0\rangle \\ \hat{N}_{(3)}^{(3)} &= N_{(3)}^{(2)} + \beta_{(3)}^{(2)} D_{(0)}^{(2)} \\ \hat{N}_{(4)}^{(3)} &= N_{(4)}^{(2)} + \beta_{(3)}^{(2)} D_{(1)}^{(2)} + \dot{Q}_{(4)}^{(2)}.\end{aligned}\tag{A.22}$$

The requirement for diagonalization through order ε^3 is that $\hat{N}_{(3)}^{(3)} = |0\rangle$. From the matrix representation, one obtains

$$q^{(2)} = \frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}, \quad r^{(2)} = \frac{3}{8}\{\varepsilon, \dot{\varepsilon}\} = \frac{3}{8}\partial\varepsilon^2/\partial x.\tag{A.23}$$

(This satisfies the pseudounitariness condition.) Thus,

$$Q^{(2)} = \left(\frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}\right)|+\rangle + \frac{3}{8}\{\varepsilon, \dot{\varepsilon}\}|-\rangle = \left(\frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}\right) = \frac{i}{2}\sigma_2 N_{(3)}^{(2)}.\tag{A.24}$$

Consequently,

$$\begin{aligned}\dot{Q}^{(2)} &= \begin{pmatrix} \frac{2}{3}\partial\varepsilon^3/\partial x - \frac{1}{8}\partial^3\varepsilon/\partial x^3 \\ \frac{3}{8}\partial^2\varepsilon^2/\partial x^2 \end{pmatrix} \\ \alpha^{(2)} &= \begin{pmatrix} [\frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}] & \frac{3}{8}[\partial\varepsilon^2/\partial x] \\ -i\frac{3}{8}\{\partial\varepsilon^2/\partial x\} & i[\frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}] \end{pmatrix} \\ \beta^{(2)} &= \begin{pmatrix} [\frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}] & i\frac{3}{8}\{\partial\varepsilon^2/\partial x\} \\ \frac{3}{8}[\partial\varepsilon^2/\partial x] & -i[\frac{2}{3}\varepsilon^3 - \frac{1}{8}\ddot{\varepsilon}] \end{pmatrix}.\end{aligned}\tag{A.25}$$

These produce the matrix representations for the terms of Eq. (A.22). The only one lacking is

$$\hat{N}_{(4)}^{(3)} = \begin{pmatrix} \frac{1}{48}[\varepsilon, [\varepsilon, \dot{\varepsilon}]] + \frac{1}{8}\{\varepsilon^2, \dot{\varepsilon}\} + \frac{3}{8}\{\varepsilon, \partial\varepsilon^2/\partial x\} + \frac{2}{3}\partial\varepsilon^3/\partial x - \frac{1}{8}\partial^3\varepsilon/\partial x^3 \\ -2\varepsilon^4 + \frac{1}{8}\{\varepsilon, \ddot{\varepsilon}\} + \frac{3}{8}\partial^2\varepsilon^2/\partial x^2 \end{pmatrix}.\tag{A.26}$$

In summary,

$$\hat{D}_{(0\cdots 4)}^{(3)} = \begin{pmatrix} \frac{1}{8}[\varepsilon, \dot{\varepsilon}] - \frac{1}{4}[\varepsilon^2, \dot{\varepsilon}] \\ -i\left(\left(\sqrt{1+2\varepsilon}\right)_{(0\cdots 4)} - \frac{1}{8}\dot{\varepsilon}^2\right) \end{pmatrix}.\tag{A.27}$$

Although the generator is diagonal through 3rd order, ($\hat{N}_{(0\cdots 3)}^{(3)} = |0\rangle$), this time it is not balanced:

$$\hat{D}_{(0\cdots 3)}^{(3)} = \begin{pmatrix} \frac{1}{8}[\varepsilon, \dot{\varepsilon}] \\ -i(\sqrt{1+2\varepsilon})_{(0\cdots 3)} \end{pmatrix} \not\propto |-\rangle. \quad (\text{A.28})$$

Balance is achieved with a block-diagonal transformation, $\hat{P}^{(2)} : \hat{G}^{(3)} \rightarrow G^{(3)}$. The only workable option is $s \sim \varepsilon^2$. (It is a straightforward though tedious matter to check that all other options, $s \sim \varepsilon^n$ with $n \neq 2$ fail.) With that, Eqs. (62) and (63) yield

$$\begin{aligned} a_{(0\cdots 4)}^{(3)} &= \hat{a}_{(3\cdots 4)}^{(3)} + [s]\hat{d}_{(1\cdots 2)}^{(3)} \\ d_{(0\cdots 4)}^{(3)} &= \hat{d}_{(0\cdots 4)}^{(3)} + \dot{s}. \end{aligned} \quad (\text{A.29})$$

To produce $a_{(0\cdots 3)}^{(3)} = 0$, we need $\hat{a}_{(3)}^{(3)} + [s]\hat{d}_{(1)}^{(3)} = 0$; i.e., $\frac{1}{8}[\varepsilon, \dot{\varepsilon}] + [s, -i\varepsilon] = 0$. From the general 2nd-order form $s = \theta\varepsilon^2 + \varphi\dot{\varepsilon}$, we find that $\varphi = i/8$. However, θ is not determined by the balance requirement (because ε^2 commutes with ε). Thus, $s = \theta\varepsilon^2 + i\frac{1}{8}\dot{\varepsilon}$, which yields $a_{(0\cdots 4)}^{(3)} = -\frac{3}{16}[\varepsilon^2, \dot{\varepsilon}]$ and $d_{(0\cdots 4)}^{(3)} = -i(\sqrt{1+2\varepsilon})_{(0\cdots 4)} + i\frac{1}{8}\dot{\varepsilon}^2 + \theta\partial\varepsilon^2/\partial x + i\frac{1}{8}\ddot{\varepsilon}$. Since the left-right symmetry requirement excludes terms of the form $\partial\varepsilon^2/\partial x$, we must have $\theta = 0$. In summary,

$$N_{(0\cdots 4)}^{(3)} = \begin{pmatrix} \frac{1}{48}[\varepsilon]^2\dot{\varepsilon} + \frac{1}{8}\{\varepsilon^2\}\dot{\varepsilon} + \frac{3}{8}\{\varepsilon\}\partial\varepsilon^2/\partial x + \frac{2}{3}\partial\varepsilon^3/\partial x - \frac{1}{8}\partial^3\varepsilon/\partial x^3 \\ -2\varepsilon^4 + \frac{1}{8}\{\varepsilon\}\ddot{\varepsilon} + \frac{3}{8}\partial^2\varepsilon^2/\partial x^2 \end{pmatrix} \quad (\text{A.30})$$

and

$$D_{(0\cdots 4)}^{(3)} = \begin{pmatrix} -\frac{3}{16}[\varepsilon^2, \dot{\varepsilon}] \\ -i(\sqrt{1+2\varepsilon})_{(0\cdots 4)} + i\frac{1}{8}\ddot{\varepsilon} + i\frac{1}{8}\dot{\varepsilon}^2 \end{pmatrix}. \quad (\text{A.31})$$

Through 3rd order, the transformed generator remains diagonal ($N_{(0\cdots 3)}^{(3)} = |0\rangle$) and is now also balanced:

$$D_{(0\cdots 3)}^{(3)} = \begin{pmatrix} -i(\sqrt{1+2\varepsilon})_{(0\cdots 3)} + i\frac{1}{8}\ddot{\varepsilon} \end{pmatrix} |-\rangle \quad (\text{A.32})$$

though, for the first time, contributions appear in it that do not belong to the Taylor series for $\sqrt{1+2\varepsilon}$.

A6. ORDER $m = 4$

The fourth step begins with a block off-diagonal transformation, $Q^{(3)} : G^{(3)} \rightarrow \hat{G}^{(4)}$, in which it is assumed that $Q^{(3)} \sim \varepsilon^4$. Since $Q^{(3)} = Q_{(4)}^{(3)}$, we have $\alpha^{(3)} = \alpha_{(4)}^{(3)}$, $\beta^{(3)} = \beta_{(4)}^{(3)}$, and $\dot{Q}^{(3)} = \dot{Q}_{(5)}^{(3)}$. With $m = 3$ in Eqs. (65) and (66) (with $G = G^{(3)}$ and $\tilde{G} = \hat{G}^{(4)}$), the $n > 0$ terms and those containing $\dot{Q}^{(3)}$ contribute nothing through 4th order, so the result is simply

$$\begin{aligned} \hat{D}_{(0\cdots 4)}^{(4)} &= D_{(0\cdots 4)}^{(3)} \\ \hat{N}_{(0\cdots 4)}^{(4)} &= N_{(4)}^{(3)} + \beta_{(4)}^{(3)}D_{(0)}^{(3)} \\ &= \hat{N}_{(4)}^{(3)} + \beta_{(4)}^{(3)}D_{(0)}^{(0)}. \end{aligned} \quad (\text{A.33})$$

The requirement for producing $\widehat{N}_{(0\dots4)}^{(4)} = |0\rangle$ is simply $\widehat{N}_{(4)}^{(3)} = i\beta_{(4)}^{(3)}|-\rangle$; i.e.,

$$\begin{aligned} q^{(3)} &= \frac{1}{2} \left(-2\varepsilon^4 + \frac{1}{8} \{\varepsilon, \ddot{\varepsilon}\} + \frac{3}{8} \partial^2 \varepsilon^2 / \partial x^2 \right) \\ r^{(3)} &= -\frac{1}{2} \left(\frac{1}{48} [\varepsilon, [\varepsilon, \dot{\varepsilon}]] + \frac{1}{8} \{\varepsilon^2, \dot{\varepsilon}\} + \frac{3}{8} \{\varepsilon, \partial \varepsilon^2 / \partial x\} + \frac{2}{3} \partial \varepsilon^3 / \partial x - \frac{1}{8} \partial^3 \varepsilon / \partial x^3 \right), \end{aligned} \quad (\text{A.34})$$

which reduces to $Q^{(3)} = \frac{i}{2} \sigma_2 \widehat{N}_{(4)}^{(3)}$. This satisfies the pseudounitariness condition, and, it would provide matrix representations for any remaining terms in Eq. (A.33); however, all of them are already represented. At this stage, the generator is diagonalized through 4th order ($\widehat{N}_{(0\dots4)}^{(4)} = |0\rangle$); however, it is still unbalanced

$$\widehat{D}_{(0\dots4)}^{(4)} = \left(\begin{array}{c} -\frac{1}{16} [\varepsilon^2, \dot{\varepsilon}] \\ -i \left(\sqrt{1+2\varepsilon} \right)_{(0\dots4)} + \frac{i}{8} (\ddot{\varepsilon} + \dot{\varepsilon}^2) \end{array} \right) \not\propto |-\rangle. \quad (\text{A.35})$$

Balance is restored with a block-diagonal transformation, $\widehat{P}^{(3)} : \widehat{G}^{(4)} \rightarrow G^{(4)}$. The form that does this is $s \sim \varepsilon^3$. (As with the previous case, other options $s \sim \varepsilon^n$ with $n \neq 3$ lead to no solution.) With $s \sim \varepsilon^3$, Eqs. (62) and (63) yield

$$\begin{aligned} a_{(0\dots4)}^{(4)} &= \widehat{a}_{(3\dots4)}^{(4)} + [s] \widehat{d}_{(1)}^{(4)} \\ d_{(0\dots4)}^{(4)} &= \widehat{d}_{(0\dots4)}^{(4)} + \dot{s}. \end{aligned} \quad (\text{A.36})$$

The requirement for $a_{(0\dots4)}^{(4)} = 0$ is simply $\widehat{a}_{(4)}^{(4)} + [s] \widehat{d}_{(1)}^{(4)} = 0$; i.e., $\frac{3}{16} [\varepsilon^2, \dot{\varepsilon}] = [\varepsilon, is]$. From the general 3rd-order form $is = \chi \varepsilon^3 + \eta \varepsilon \dot{\varepsilon} + \psi \dot{\varepsilon} \varepsilon + \theta \ddot{\varepsilon}$, we find that θ must vanish and that $\psi = \eta = 3/16$, although χ remains undetermined (because $[\varepsilon, \varepsilon^3] = 0$). Thus, $is = \chi \varepsilon^3 + \frac{3}{16} \{\varepsilon, \dot{\varepsilon}\}$ and $i\dot{s} = \chi \partial \varepsilon^3 / \partial x + \frac{3}{8} \dot{\varepsilon}^2 + \frac{3}{16} \{\varepsilon, \ddot{\varepsilon}\}$. However, left-right symmetry requires $\chi = 0$ to eliminate the $\partial \varepsilon^3 / \partial x$ term. Thus, through 4th order, the transformed generator remains diagonal ($\widehat{N}_{(0\dots4)}^{(4)} = |0\rangle$) and is also balanced:

$$D_{(0\dots4)}^{(4)} = \left(-i \left(\sqrt{1+2\varepsilon} \right)_{(0\dots4)} + i \frac{1}{8} \ddot{\varepsilon} - i \frac{1}{4} \dot{\varepsilon}^2 - i \frac{3}{16} \{\varepsilon, \ddot{\varepsilon}\} \right) |-\rangle. \quad (\text{A.37})$$

The contributions that do not belong to the Taylor series for $\sqrt{1+2\varepsilon}$ include the 3rd-order one that persists from the previous step and a pair of new 4th-order terms.